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Elastic scattering of electrons and positrons by helium atom

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Calculations of differential and total cross sections for the elastic scattering of electrons and positrons by neutral helium atom have been performed over the range of impact energies 50–700 eV employing the Schwinger variational principle for scattering amplitude. The Hartree-Fock static potential for helium atom has been used in the calculations. The results are compared with the Born approximation calculations and also with experimental findings.

INTRODUCTION

In the present paper calculations are carried out for the differential and total cross sections of the elastically scattered electrons by helium atom for various energies between 50 and 700 eV, the effects of exchange and polarization are considered to be not so important. The corresponding results for positron scattering are also reported.

Experimental measurements on the elastic collision between electrons and helium atoms have been carried out by several workers (Hughes *et al* 1932, Werner 1933, Vriens *et al* 1968, Bromberg 1969) over a wide range of electron impact energies. A number of theoretical investigations have also been made on the e—He elastic scattering. The calculation of scattering cross sections of high energy electrons by helium atom has been performed by Mukherjee (1961) in Born approximation where the use of a refined wave function which includes the correlation function depending on the mutual distance of the atomic electrons has been made. Kim & Inokuti (1968) have used the twenty-term Hylleraas wave function of Hart & Herzberg (1957) in their Born-approximation calculations. Here we apply the Schwinger variational principle for the scattering amplitude (Lippman & Schwinger 1950) to the same collision problem. The static field of helium atom is represented by a linear combination of several Yukawa potentials (Tietz 1965). The form of the trial wave function taken by us has been previously used by Mower (1955) for the calculation of differential cross section in the elastic scattering of electrons from neon atom where it has yielded results very close to the numerical solution.

Unlike other variational principles, Schwinger principle does not require that the trial functions involved should have a particular asymptotic form. This principle has been put in two forms. In one, by making the usual expansions in spherical harmonics an infinite set of independent integral equations and hence a corresponding set of variational expressions for the phase shifts has been obtained, while in the other, the entire scattering amplitude has been expressed in a stationary form. The calculation of scattering cross section by summing over the individual phase shifts, though accurate, involves a lot of numerical computations, whereas the calculation by the direct estimation of scattering amplitude is intrinsically much simpler.

The choice of the potential as a linear combination of several Yukawa potentials is motivated by the fact that for this potential the integrals occuring in the variational principle can be evaluated in closed form for some suitable trial functions This evaluation is possible for the relatively simple form of the Fourier transform of the Yukawa potential. For other potentials the variational formulation may not yield closed form expressions for the scattering amplitudes Unless the integrals can be evaluated in closed form, computations using the Schwinger variational formulation become very tedious and have practically no advantage over exact numerical integration of the differential equation.

Mathematical formulation

The scattering of a particle of mass m by a potential $V(\vec{r})$ is described by an exact solution to the integral equation(Mott & Massy 1965)

$$\psi_i(\vec{r}) = e^{i\vec{k}_i\cdot\vec{r}} + \frac{2m}{\hbar^2} \int G(\vec{r}, \vec{r}')V(\vec{r}')\psi_i(\vec{r}')d\vec{r}', \tag{1}$$

where

$$G(\vec{r}, \vec{r}') = -\frac{1}{4\pi}\frac{e^{ik|r-r'|}}{|r-r'|}$$

is the free space Green function for the Helmholtz equation and $E = \hbar^2k^2/2m$ is the energy of the incident particle. The vector $\vec{k_i} = k\,\hat{n}_i$, where the unit vector $\hat{n}_i$ specifies the direction of incidence and the vector $\vec{r} = r\hat{n}$ is the radius vector which specifies the position of the particle The amplitude for the scattering from direction $\hat{n}_1$ to direction $-\hat{n}_2$ is defined by

$$f(\hat{n}_1,-\hat{n}_2) = -\frac{1}{4\pi}\int e^{ik\hat{n}_2\cdot r'}\; U(r')\psi_1(r')dr',$$

where

$$U(\vec{r}) = 2mV(\vec{r})/\hbar^2.$$

For the approximate determination of the scattering amplitude by the Schwinger variational method we take, following Mower (1955), the functional for the scattering amplitude as

$$[f(\hat{n}_1, -\hat{n}_2)] = -\frac{1}{4\pi}\Big[\int e^{ik\hat{n}_2\cdot\vec{r}}\; U(\vec{r})\psi_1(\vec{r})d\vec{r} + \int e^{ik\hat{n}_1\cdot\vec{r}}\; U(\vec{r})\psi_2(\vec{r})d\vec{r}$$
$$-\int \psi_2(\vec{r})U(\vec{r})\psi_1(\vec{r})d\vec{r} + \int\int \psi_2(\vec{r})U(\vec{r})G(\vec{r}, \vec{r}')U(\vec{r}')\psi_1(\vec{r}')d\vec{r}d\vec{r}'\Big] \quad \ldots \tag{2}$$

where ψ_1 and ψ_2 are trial solutions of (1). Using trial functions of the form

$$\psi_i = C_1 e^{ik\hat{n}_i.\vec{r}} + C_2 e^{-ik\hat{n}_i.\vec{r}}, \quad i = 1, 2$$

the expression (2) for the scattering amplitude is obtained as

$$[f(\hat{n}_1, -\hat{n}_2)] = 2C_1 f_{b1}(\hat{n}_1, -\hat{n}_2) + 2C_2 f_{b1}(\hat{n}_1, \hat{n}_2)$$
$$-(C_1^2+C_2^2)[f_{b1}(\hat{n}_1, -\hat{n}_2) - f_{b2}(\hat{n}_1, -\hat{n}_2)] - 2C_1C_2[f_{b1}(\hat{n}_1, \hat{n}_2) - f_{b2}(\hat{n}_1, \hat{n}_2)], \quad \ldots \quad (3)$$

where

$$f_{b1}(\hat{n}_1, -\hat{n}_2) = -\frac{1}{4\pi} \int e^{ik(\hat{n}_1+\hat{n}_2).\vec{r}}\, U(\vec{r}) d\vec{r} = (-\vec{k}_2 \,|\, U \,|\, \vec{k}_1)$$

$$f_{b2}(\hat{n}_1, -\hat{n}_2) = -\frac{1}{4\pi} \int\int e^{ik(\hat{n}_1.\vec{r}'+\hat{n}_2.\vec{r})}\, U(\vec{r}) G(\vec{r}, \vec{r}') U(\vec{r}') d\vec{r} d\vec{r}' \quad \ldots \quad (4)$$

$$= \frac{4\pi}{(2\pi)^3} \int \frac{(-\vec{k}_2 \,|\, U \,|\, \vec{\eta})(\vec{\eta} \,|\, U \,|\, \vec{k}_1)}{\eta^2 - k^2} d\vec{\eta}$$

are, respectively, the first and second terms in the Born series of approximations to the scattered amplitude. Substituting

$$f_{b1}(\hat{n}_1, \hat{n}_2)/f_{b1}(\hat{n}_1, -\hat{n}_2) = \lambda \text{ and } f_{b2}(\hat{n}_1, -\hat{n}_2)/f_{b1}(\hat{n}_1, -\hat{n}_2) = \mu(\hat{n}_1, -\hat{n}_2)$$

the expression (3) may be rewritten as

$$[f(\hat{n}_1, -\hat{n}_2)] = f_{b1}(\hat{n}_1, -\hat{n}_2)[2C_1 + 2C_2\lambda - (C_1^2+C_2^2)(1-\mu(\hat{n}_1, -\hat{n}_2))$$
$$-2C_1C_2\lambda(1-\mu(\hat{n}_1, \hat{n}_2))]$$

Now, adjusting the parameters according to the conditions

$$\partial[f]/\partial C_i = 0, \quad i = 1, 2$$

the scattering amplitude is given by

$$[f(\hat{n}_1, -\hat{n}_2)] = f_{b1}(\hat{n}_1, -\hat{n}_2)[(1+\lambda^2)(1-\mu(\hat{n}_1, -\hat{n}_2)) - 2\lambda^2(1-\mu(\hat{n}_1, \hat{n}_2))]/$$
$$[(1-\mu(\hat{n}_1, -\hat{n}_2))^2 - \lambda^2(1-\mu(\hat{n}_1, \hat{n}_2))^2 \quad \ldots \quad (5)$$

The Hartree—Fock screening factor (Tietz 1965) for neutral atoms can be expressed analytically in the form

$$f(r) = \sum_i \alpha_i e^{-\gamma_i r} \quad (6a)$$

so that the electrostatic scattering potential may be written as

$$V(r) = \frac{Ze^2}{r} f(r). \quad (6b)$$

With this potential the first and second Born scattering amplitudes are obtained from (4) as (Morse & Feshback 1953, Lewis 1956)

$$f_{b1}(\hat{n}_1, -\hat{n}_2) = -\frac{2mZ}{\hbar^2}\sum_i \frac{\alpha_i}{\gamma_i^2+4k^2\sin^2\frac{\theta}{2}}$$

$$f_{b2}(\hat{n}_1, -\hat{n}_2) = \frac{4\pi}{(2\pi)^3}\left(\frac{2mZ}{\hbar^2}\right)^2 \sum_{i,j} \frac{\alpha_i\alpha_j}{k^3} M(\gamma_i, \gamma_j) \qquad \dots (7)$$

where

$$ReM(\gamma_i, \gamma_j) = \frac{2\pi^2k^3T}{T^2+S^2}, \quad \theta = 0 \text{ and } i = j$$

$$= \frac{\pi^2k^3}{R}\left[\tan^{-1}\frac{S+R}{T} - \tan^{-1}\frac{S-R}{T}\right], \quad \text{otherwise}$$

and

$$I_mM(\gamma_i, \gamma_j) = \frac{2\pi^2k^3S}{T^2+S^2}, \quad \theta = 0 \text{ and } i = j$$

$$= \frac{\pi^2k^3}{R}\,\frac{1}{2}\ln\cdot\frac{T^2+(R+S)^2}{T^2+(R-S)^2}, \quad \text{otherwise}$$

with

$$R = [k^2(K^2+\gamma_i^2+\gamma_j^2)^2 - P^2\gamma_i^2\gamma_j^2]^{\frac{1}{2}}$$

$$S = k[K^2+(\gamma_i+\gamma_j)^2], \quad T = \gamma_i\gamma_j(\gamma_i+\gamma_j)$$

$$\vec{K} = \vec{k}_1+\vec{k}_2, \quad \vec{P} = \vec{k}_1-\vec{k}_2, \quad \theta = \arccos(\hat{n}_1.(-\hat{n}_2)).$$

Using the equations (7) and the definitions of λ, μ, we can determine the scattering amplitude from the expression (5) and hence the differential cross-sections for the scattering of particles by an atom. The total scattering cross-section Q may be obtained by integration of the differential cross-section through solid angle or by employing the optical theorem

$$Q = \frac{4\pi}{k} I_m f(\hat{n}_1, \hat{n}_1).$$

Results and discussion

We have calculated the differential and total cross-sections of elastically scattered electrons and positrons having incident energy between 50 and 700 eV by the Schwinger variational method and the Born approximation. Integrations over angles yielding total cross-sections have been performed numerically by Simpson's rule with suitable intervals. The parameters occurring in the expression for the potential (c.f. equations 6a and 6b), which reproduces the Hartree-Fock field of helium atom, are

$\alpha_1 = 1.0000$, $\alpha_2 = -0.6195$ $\alpha_3 = -0.1846$, $\alpha_4 = 0.6195$, $\alpha_5 = 0.1846$

$\gamma_1 = 2.4907$ $\gamma_2 = 3.8530$ $\gamma_3 = 6.1212$, $\gamma_4 = 2.8530$, $\gamma_5 = 5.1212$

The results of our calculation for the differential cross sections are shown in figure 1. We compare our results for the electron scattering for 50 eV and 700

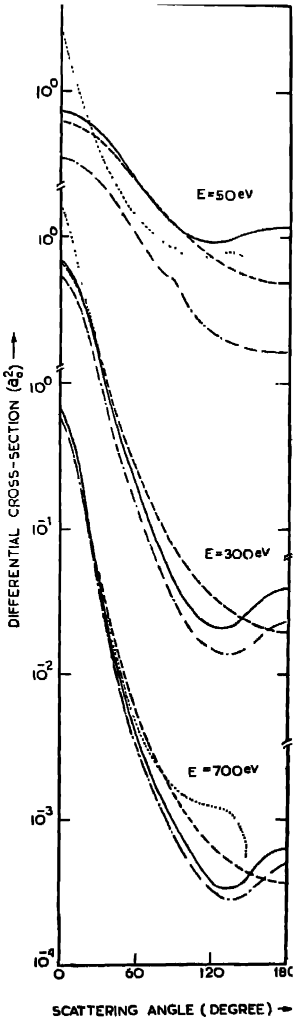

Figure 1. .... experimental findings for electron scattering.
- - - - - - Born results
———— variational calculation for electron scattering
· — · — variational calculation for positron scattering.

eV with the experimental data of Hughes *et al* (1932) and that for 300 eV with the experimental data of Vriens *et al* (1968).

At high energies the results for the differential cross-section for electron and positron scattering are nearly the same. But with the decrease of energy there is a marked difference between the two results, as expected. The results for the differential cross-sections for electron scattering obtained by variational calculations are in slightly better agreement with experiment than those calculated by Born-approximation at all energies. In the high energy region ($E \geqslant 600$ eV) our theoretical results for the differential cross-sections agree well with the experimental findings for all scattering angles, which contribute appreciably to the total cross-section. For small angle of scattering the ratio of the experimental findings and the corresponding Born results for the differential cross-sections is quite large, more so for low incident energy. In the incident energy region of 300 eV and above, for larger angles, this ratio decreases below unity with the increase of angle. Again with further increase of scattering angle the value of the ratio gradually increases and finally becomes greater than unity. This character is also maintained in the variational calculation.

We obtain the total cross sections for the systems in two ways, by the integration of differential cross sections over the solid angle and by using the optical theorem. In table 1, we have presented these two results of total cross-sections

TABLE 1 Total cross sections Q (in units of πa_0^2, where a_0 is the Bohr radius) for elastic scattering of electrons and positrons by helium atom

Incident energy (eV)	Q^*	Q (Born)	Q^{**}		Q^{***}	
			electrons	positrons	electrons	positrons
50		0.711005	0.8043	0.3131	0.89298	0 35745
100	0.762	0.410395	0 4063	0.2204	0.46267	0 2672015
150	0 443	0 287944	0.2767	0.1742	0 31380	0 21207
200	0.308	0.221654	0.2111	0.1453	0.23731	0 17507
300	0.190	0.1516999	0.1440	0.1095	0.15929	0 12914
400	0.142	0.1152831	0.1096	0.8823×10^{-1}	0.11976	0.102044
500		0.929577×10^{-1}	0.8868×10^{-1}	0.7415×10^{-1}	0.95901×10^{-1}	$0\ 842613\times10^{-1}$
600		0.778729×10^{-1}	0.7454×10^{-1}	0.6394×10^{-1}	0.79957×10^{-1}	0.71729×10^{-1}
700		$0\ 669988\times10^{-1}$	0.6434×10^{-1}	0.5627×10^{-1}	0.68549×10^{-1}	0.62427×10^{-1}

*Experimental results of Vriens *et al* (1968)

**Calculated from the variationally obtained differential cross-sections by integration through the solid angle

***Calculated from the variationally obtained amplitude by using the optical theorem and the corresponding Born results and compared them with the experimental findings of Vriens *et al* (1968) It is seen from the table that at 100 eV and above the cross sections obtained by integration are nearly equal to the Born cross-sections, but the cross-sections obtained by employing the optical theorem are always greater than these two results and closer to experimental findings.

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